

Possible π -phase shift at interface of two pnictides with antiphase s-wave pairingWei-Qiang Chen and Fu-Chun Zhang¹¹*Department of Physics and Center of Theoretical and Computational Physics,
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We examine the nature of Josephson junction between two identical Fe-pnictides with anti-phase s-wave pairing. π -phase shift is found if the junction barrier is thick and the two Fe-pnictides are oriented in certain directions relative to the interface. Our theory provides a possible explanation for the observed half integer flux quantum transitions in a niobium/polycrystal NdFeAsO loop, and attributes the π -phase shift to intergrain junctions of Fe-pnictides.

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Since the discovery of a new class of unconventional superconductors based on *Fe* compounds, their pairing symmetry has been one of the most interesting issues. Different from the high T_c cuprates, where the pairing symmetry is universally d-wave, there are experimental evidences that pairing symmetry in the iron pnictides may not be universal. The superconductors with higher transition temperature T_c are supported by spin singlet s-wave¹⁻⁴, while LaFePO with lower T_c seems to have nodal in its gap function⁵. It is interesting to note that the iron pnictide has both hole and electron Fermi pockets, and the predicted s-wave pairing state has superconducting order parameters with opposite signs on the electron and hole pockets, often called anti-phase s-wave or s_{\pm} -wave state⁶⁻¹¹. Among the experiments in support of the s_{\pm} pairing state, the phase sensitive experiment reported by Chen et al.⁴ provides the most convincing evidence, where they observed integer and half integer flux quantum transitions in a niobium/polycrystal NdFeAsO loop. The observed half integer flux quantum demonstrates the existence of π -junctions in the loop of niobium and polycrystal pnictides, hence a direct evidence for the opposite signs of the superconducting order parameters in different Fermi pockets. In passing, we recall that phase sensitive experiments provided a direct evidence for the $d_{x^2-y^2}$ pairing in superconducting cuprates^{12,13}.

Because of the polycrystal nature in the sample of the NdFeAsO, a phase shift of π in the composite loop in tunneling could occur at the Nb-Nd-1111 interface, or at the junction between two Nd-1111 grains⁴. Theoretically, there have been several studies to examine the possible π -phase shift involving an interface between a conventional superconductor and a Fe-pnictide with s_{\pm} pairing under certain conditions¹⁴⁻¹⁶, which may help understand the possible π -junction at the Nb-Nd-1111 interface. The possibility of a π -phase shift in the interface of two Fe-pnictide intergrains of the same doping has not been carefully examined, although intuitively one may consider it unlikely. In this paper, we study a Josephson junction between two iron pnictides. When the junction barrier is thick and the two Fe-pnictide grains are oriented in certain directions relative to the interface, the junction could give a π -phase shift.

The π -junction is a Josephson junction with negative

critical current, and the critical current for junction between conventional superconductors is defined as

$$I_c \propto \int d\mathbf{k} d\mathbf{q} \frac{|T|^2 \Delta_1(\mathbf{k}) \Delta_2(\mathbf{q})}{E_1(\mathbf{k}) E_2(\mathbf{q}) [E_1(\mathbf{k}) + E_2(\mathbf{q})]}, \quad (1)$$

where $T_{\mathbf{k}\mathbf{q}}$ is the tunneling matrix, $E_i(\mathbf{k}) = \sqrt{\epsilon_i(\mathbf{k})^2 + \Delta_i(\mathbf{k})^2}$ is the quasiparticle energy of the superconductor $i = 1, 2$ respectively, $\epsilon_i(\mathbf{k})$ is the single electron energy measured relative to the chemical potential, and $\Delta_{1(2)}$ are superconducting gap functions, which we shall assume to be real here. The co-efficient of the integral will always be taken to be positive throughout this paper. Eq. (1) can be easily generalized to the iron pnictide superconductors with multi-bands, and the critical current are given by,

$$I_c \propto \sum_{\alpha\beta} \int d\mathbf{k} d\mathbf{q} \frac{|T_{\mathbf{k}\mathbf{q}}^{\alpha\beta}|^2 \Delta_1^{\alpha}(\mathbf{k}) \Delta_2^{\beta}(\mathbf{q})}{E_1^{\alpha}(\mathbf{k}) E_2^{\beta}(\mathbf{q}) [E_1^{\alpha}(\mathbf{k}) + E_2^{\beta}(\mathbf{q})]}, \quad (2)$$

where α and β are index of bands, and all other notations are the same as in the single band expression except for the additional band indices. As pointed out by Sigrist and Rice¹⁷, though the critical current is not gauge invariant, the parity of the number of the π -junctions in a loop is gauge invariant. So in the following, we choose a convenient gauge where the gap functions of the hole pockets are positive and the gap functions of the electron pockets are negative.

In the usual case, the junction between two identical superconductors is a 0-junction with I_c to be positive. Let us consider a point junction of two identical pnictide superconductors. In this case, $T_{\mathbf{k}\mathbf{q}}^{\alpha\beta} = t_0$, independent of crystal momentum and the band. The critical current is found to be

$$I_c \propto \sum_{\alpha\beta} \int d\mathbf{k} d\mathbf{q} \frac{\Delta_1^{\alpha}(\mathbf{k}) \Delta_2^{\beta}(\mathbf{q})}{E_1^{\alpha}(\mathbf{k}) E_2^{\beta}(\mathbf{q}) [E_1^{\alpha}(\mathbf{k}) + E_2^{\beta}(\mathbf{q})]}. \quad (3)$$

According to Ambegaokar and Baratoff, the above formula can be further written as

$$I_c \propto \sum_{\alpha\beta} \text{sgn}(\Delta_{\alpha} \Delta_{\beta}) N_{\alpha} N_{\beta} \Delta_m K \left(\sqrt{1 - \frac{\Delta_m^2}{\Delta_M^2}} \right), \quad (4)$$

where N_α is the density of states of Fermi pocket α , $\Delta_m = \min(|\Delta^\alpha|, |\Delta^\beta|)$ and $\Delta_M = \max(|\Delta^\alpha|, |\Delta^\beta|)$ are the smaller and larger gap on the two pockets respectively, and K is the elliptical integral. In the special case, all the gap functions have the same amplitude, the elliptical function $K(0) = \pi/2$, so that $I_c \propto (\sum_\alpha \text{sgn}(\Delta_\alpha) N_\alpha)^2 > 0$. This positive definiteness appears to remain valid when the gap amplitudes are different. In particular we consider below iron based superconductor in the 2-dimension limit. We shall work in extended Brillouin zone for convenience and set the Fe-Fe distance to be length unit. There are two electron Fermi pockets with one around $(\pi, 0)$ and one around $(0, \pi)$, and two hole Fermi pockets around $(0, 0)$ point. We consider the case, where the superconducting gaps on one of the hole pockets and on the electron pockets are about the same while the gap on another hole pocket is smaller, as reported in ARPES for BaFe_2As_2 ¹⁹. By using the properties of the elliptical function, $\sqrt{1-k^2}K(k) \leq K(0) = \frac{\pi}{2}$, the critical current I_c is found to be always positive. This illustrates that the different signs of the s -wave gap functions is necessary condition, but not sufficient condition for a π -junction. Below we shall examine a thick barrier junction between two pnictide superconductors of certain orientation and show that such a junction may give a π -phase shift.

We consider two half-infinite iron pnictide samples separated by a vacuum barrier with height U and width d as shown in fig. 1. The interface is along yz plane so that the momentum components along y and z directions are conserved in the tunneling process. For a thick barrier, the usual assumption that the tunneling matrix element T is independent of momentum or crystal momentum is no longer valid. This can be illustrated by examining the free electron tunneling process in quasi one-dimension, where $|T|^2$ is the transmission coefficient of the scattering problem. For a potential barrier normal to x direction with height U and length d , the transmission coefficient reads

$$|T|^2 = \frac{4\kappa^2 k_x q_x}{\kappa^2(k_x + q_x)^2 + (\kappa^2 + k_x^2)(\kappa^2 + q_x^2) \sinh^2(\kappa d)}, \quad (5)$$

where k_x and q_x are the x -direction wavevector of the incoming and outgoing plane waves respectively, κ is the imaginary wavevector inside the barrier with $\kappa = \frac{1}{\hbar} \sqrt{2m(U-E) + \hbar^2 k_\parallel^2}$, m is the mass of the electron, and k_\parallel is the wavevector parallel to the barrier interface, which is conserved in the scattering process. In the thick barrier limit, i.e. $\kappa d \gg 1$, one have

$$|T|^2 \simeq \frac{16\kappa^2 k_x q_x}{(\kappa^2 + k_x^2)(\kappa^2 + q_x^2)} e^{-2\kappa d}. \quad (6)$$

If we assume that $p \equiv \frac{1}{\hbar} \sqrt{2m(U-E)} \gg k_\parallel$, it can be further simplified as

$$|T|^2 \propto \frac{\kappa^2 k_x q_x}{(\kappa^2 + k_x^2)(\kappa^2 + q_x^2)} e^{-\frac{\kappa^2}{p} d}, \quad (7)$$

so the transmission coefficient decays exponentially with the increment of planar wave-vector k_\parallel . The above formula can be extended to the electron tunneling process in a lattice with the following modifications as pointed out by Mazin¹⁸. All the wave-vectors in the expression of the above equation are replaced by the corresponding group velocities except k_\parallel in the exponential factors which tracks the oscillation of the wavefunction parallel to the interface direction. The second modification is to replace the plane wavefunction in the free electron case by a Bloch wave $\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \omega_{n\mathbf{k}}(\mathbf{r})$. The periodical function $\omega_{n\mathbf{k}}$ can be further Fourier's transformed as $\omega_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{K}} F_{n\mathbf{k},\mathbf{K}} e^{i\mathbf{K}\cdot\mathbf{r}}$, where \mathbf{K} is reciprocal lattice vector. If $\omega_{n\mathbf{k}}(\mathbf{r})$ is localized, one can approximate $F_{n\mathbf{k},\mathbf{K}} \sim \text{constant}$ for not very large \mathbf{K} . The wavefunction can finally be written as

$$\psi_{n\mathbf{k}}(\mathbf{r}) = F_{n\mathbf{k}} \sum_{\mathbf{K}} e^{i(\mathbf{k}+\mathbf{K})\cdot\mathbf{r}}. \quad (8)$$

According to eqn. (7), the tunneling is mainly from the component with $K_\parallel = 0$, so the tunneling matrix reads

$$|T_{\mathbf{k}\mathbf{q}}^{\alpha\beta}|^2 \propto A_{\alpha\mathbf{k},\beta\mathbf{q}} \sum_{\mathbf{K},\mathbf{Q}} 4m^2 \hbar^2 \kappa^2 \delta_{(\mathbf{k}+\mathbf{K})_\parallel, (\mathbf{q}+\mathbf{Q})_\parallel} \times \frac{v_{\alpha\mathbf{k}x} v_{\beta\mathbf{q}x}}{(\hbar^2 \kappa^2 + m^2 v_{\alpha\mathbf{k}x}^2)(\hbar^2 \kappa^2 + m^2 v_{\beta\mathbf{q}x}^2)} e^{-\frac{(\mathbf{k}+\mathbf{K})_\parallel^2}{p} d}, \quad (9)$$

where \mathbf{K} and \mathbf{Q} are the reciprocal lattice vector of FeAs sample 1 and 2 respectively, $\kappa = \frac{1}{\hbar} \sqrt{2m(U-E) + \hbar^2 (\mathbf{k}+\mathbf{K})_\parallel^2}$, the delta function tracks the planar momentum conservation, A is a factor related to the detail information of the electron wavefunction and can usually be approximated as constant, and $v_{\alpha\mathbf{k}x}$ and $v_{\beta\mathbf{q}x}$ are the group velocity along x direction of the electron in band $\alpha(\beta)$ with lattice wavevector $\mathbf{k}(\mathbf{q})$ respectively.

The exponential factor in above equation can be rewritten as $e^{-\frac{\kappa^2}{p} d} e^{-\frac{(2\mathbf{k}+\mathbf{K})_\parallel \cdot \mathbf{K}_\parallel}{p} d}$, where the first term is the contribution of the Brillouin zones with $K_\parallel = 0$ and the second term is the additional factor for the Brillouin Zones with finite K_\parallel . In the following, we ignore the z -axis dispersion, which is very weak in 1111 compound, and only consider the physics of FeAs plane. For the configuration shown in fig. 1, we have that $K_y = 2n\pi/a$ for FeAs sample 1 and $Q_y = \sqrt{2}m\pi/a$ for FeAs sample 2, where a is the lattice constant. For a barrier with $d \sim 10a$ and $p \equiv \frac{1}{\hbar} \sqrt{2m(U-E)} \approx 10\pi/a$, the largest factor for Brillouin zone with finite K_\parallel is $e^{-2\pi} \approx 0.002$. So only the contribution from the Brillouin Zone with $K_\parallel = 0$ is important. And because $p^2 \gg k_\parallel^2$, eqn. (7) becomes

$$|T_{\mathbf{k}\mathbf{q}}^{\alpha\beta}|^2 \propto \delta_{k_y, q_y} v_{\alpha\mathbf{k}x} v_{\beta\mathbf{q}x} e^{-\frac{\kappa^2}{p} d}. \quad (10)$$

Because of the fast drop of the coherence factor $\frac{\Delta}{2E}$ in the critical current when the state is away from the

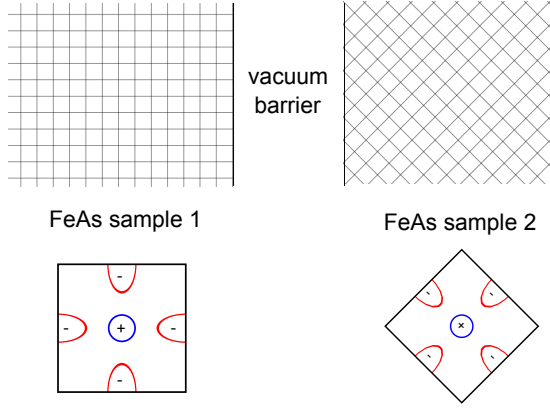


FIG. 1: Schematic diagram of a thick Josephson junction of two iron pnictides separated by a vacuum. The Fe lattice orientation for the two materials are depicted in the upper panel. Lower panel is the corresponding Fermi surface in the Brillouin zone for the two material.

Fermi surface, the planar momentum conservation parallel to the interface, and the exponential factor in tunneling matrix in eqn. (10), only the electron pockets around X and the hole pockets of iron pnictide sample 1 and the hole pockets of sample 2 are important in the configuration shown in Fig. 1. Because $\mathbf{k}_{\parallel} \sim 0$, the exponential factor in eqn. (10) becomes a constant. For simplicity, we assume that the gap Δ is momentum independent which is consistent with the ARPES result². By substituting eqn. (10) into eqn. (2) and noticing that velocity $v_x \propto \frac{\partial \epsilon}{\partial k_x}$, the critical current reads

$$I_c \propto \sum_{\alpha\beta} \int dk_y \int_{\epsilon_m^{\alpha}(k_y)}^{\epsilon_M^{\alpha}(k_y)} d\epsilon_1 \int_{\epsilon_m^{\beta}(k_y)}^{\epsilon_M^{\beta}(k_y)} d\epsilon_2 \frac{\Delta_1^{\alpha} \Delta_2^{\beta}}{E_1^{\alpha} E_2^{\beta} [E_1^{\alpha} + E_2^{\beta}]}, \quad (11)$$

where $\epsilon_m^{\alpha}(k_y)$ and $\epsilon_M^{\alpha}(k_y)$ are the minimum and maximum energy of the electron in band α with given k_y and any k_x . If $\epsilon_m^{\alpha(\beta)}(k_y) - E_f \ll -\Delta_{\alpha(\beta)}$ and $\epsilon_M^{\alpha(\beta)}(k_y) - E_f \gg \Delta_{\alpha(\beta)}$, the integral can be approximated with $\text{sgn}(\Delta_{\alpha}\Delta_{\beta})\Delta_m K(\sqrt{1 - \Delta_m^2/\Delta_M^2})$, where Δ_m and Δ_M are the smaller one and larger one of amplitude of the two gaps Δ_{α} and Δ_{β} . If the amplitude of the superconducting gap on those bands are very close to each other, the elliptical integral K can be approximated as a constant, and the final result is

$$I_c \propto \sum_{\alpha\beta} \text{sgn}(\Delta_{\alpha}\Delta_{\beta})\Delta_m \min(\lambda_{1\alpha}, \lambda_{2\beta}), \quad (12)$$

where $\lambda_{i\gamma}$ is the width along the direction parallel to the interface of the Fermi pocket γ of FeAs sample i .

Then we consider the real materials. Most iron-based superconductors in 1111 family are electron doped including the material used in the experiment by Chen et al.⁴ The theoretical calculations and experiments show that the parent compound have two hole pockets around

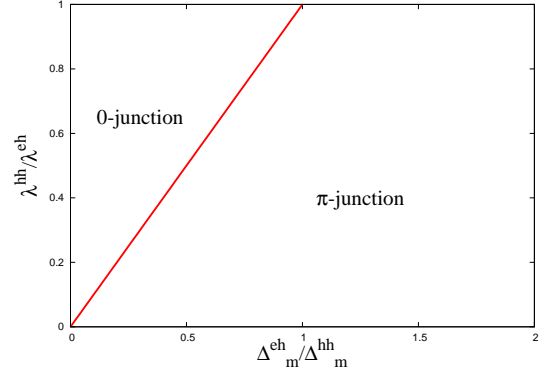


FIG. 2: The type of Josephson junction. The red solid line is $\lambda^{hh}/\lambda^{eh} = \Delta_m^{eh}/\Delta_m^{hh}$ which separate the two regions. See text for details.

Γ point and one electron pockets around X point. After doping of the electrons, one would expect the electron pocket expands and the hole pockets shrink. when the electron concentration is large enough, the inner hole pocket will be too small to contribute to the critical current or even vanished. In this case, eqn. (12) becomes

$$I_c \propto \Delta_m^{hh} \lambda^{hh} - \Delta_m^{eh} \lambda^{eh}, \quad (13)$$

where $\Delta_m^{\alpha\beta} = \min(|\Delta_{1\alpha}|, |\Delta_{2\beta}|)$, $\lambda^{\alpha\beta} = \min(\lambda_{1\alpha}, \lambda_{2\beta})$. So the Josephson junction is a π -junction when $\lambda^{hh}/\lambda^{eh} < \Delta_m^{eh}/\Delta_m^{hh}$ and vice versa, as shown in fig. 2. The ARPES experiment has shown that the gaps on electron pockets and the outer hole pocket are same², i.e. $\Delta_m^{hh} = \Delta_m^{eh}$. So the sign of the critical current is determined by the width of the Fermi pockets along the direction parallel to the interface. The DFT result of *LaFeAsO* has suggest that the hole pocket has a little anisotropy and the Fermi wavevector along (110) direction is a little larger than the one along (100) direction²⁰, i.e. $\lambda_1^h < \lambda_2^h$ and $\lambda^{hh} = \lambda_1^h$. On the other hand, if the electron concentration is large enough, one should have that the width of the electron pocket is larger than the one of the hole pocket, i.e. $\lambda_1^e > \lambda_2^h$ and $\lambda^{eh} = \lambda_2^h > \lambda^{hh}$, which indicates that the junction is a π -junction. Another possibility is that the electron concentration of sample 1 is a littler larger than the one of sample 2. In this case, the size of hole pocket of sample 1 should be smaller than the one of sample 2, i.e. $\lambda_1^h < \lambda_2^h$. Again, if the electron concentration is large enough, one should have $\lambda_1^e > \lambda_2^h$, and the junction should also be a π -junction.

For the material in 122 family, both electron and hole can be doped with various ways. For the electron doped 122 material, the ARPES experiment suggests that there is only one hole pocket around Γ point, and the widths of hole pocket and electron pocket are comparable¹⁹ which should be similar with the e-doped 1111 case. So one should observe similar phenomena in the e-doped 122 material with large enough electron doping. But the situation is different in the hole doped case where both of

the two hole pockets will contribute to the critical current, and the size of hole pockets should be larger than the one of electron pocket. By taking account that the gap on outer hole pocket is same as the one on electron pocket, one can find that the critical current is positive according to eqn. (12), and one can not observe half-flux jump in those hole doped 122 material.

In summary, we have examined the Josephson junctions between two Fe-pnictides with the same electron concentration. We found that it is impossible for two

Fe-pnictides to form a π -junction in the case that tunneling matrix element is momentum independent. But a π -junction can be formed in the thick barrier case where the pockets with large parallel momentum are irrelevant. Such π -junctions may be the origin of the π -flux jump in C.-T. Chen et al.'s experiment.

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